

1,1,2,2-Tetrafluoro-2-(1,1,2,2-tetrafluoroethoxy)ethane-1-sulfonyl fluoride
104729-49-9 | DTXSID40446988

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 71.4 °C

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 7.01e-01

Nearest Neighbors from the Training Set

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3,3,4,4,5,5-Hexafluorodihydro-
2H-pyran-2,6(3H)-dione

Measured: 72.0

Predicted: 74.7

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Trifluoromethanesulphonyl
chloride

Measured: 30.5

Predicted: 36.6

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Cyclohexene, 1,2-
dichlorooctafluoro-

Measured: 113

Predicted: 109

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2,4-Pentanedione, 1,1,1,5,5,5-
hexafluoro-

Measured: 70.0

Predicted: 67.8